Ferromagnetism in the Hubbard model with a generalized type of hopping

Pavol Farkašovský
Institute of Experimental Physics, Slovak Academy of Sciences
Watsonova 47, 043 53 Košice, Slovakia

Abstract

The extrapolation of small-cluster exact-diagonalization calculations is used to examine ferromagnetism in the one-dimensional Hubbard model with a generalized type of hopping. It is found that the long-range hopping with power decaying hopping amplitudes ($t_{ij} \sim q^{|i-j|}$) stabilizes the ferromagnetic state for a wide range of electron interactions U and electron concentrations n. The critical value of the interaction strength $U_c(q)$ above which the ferromagnetic state becomes stable is calculated numerically and the ground-state phase diagram of the model (in the U-q plane) is presented for physically the most interesting cases.

The Hubbard model has become, since its inception [1] in 1963, one of the most popular examples of a system of interacting electrons with short-range interactions. It has been used in the literature to study a great variety of many-body effects in metals, of which ferromagnetism, metal-insulator transitions, charge-density waves and superconductivity are the most common examples. Of all these cooperative phenomena the problem of ferromagnetism in the Hubbard model has the longest history. Although the model was originally introduced to describe the band ferromagnetism of transition metals, it soon turned out that the single-band Hubbard model is not the canonical model for ferromagnetism. In fact the existence of saturated ferromagnetism has been proven rigorously only for very special limits. The first well-known example is the Nagaoka ferromagnetism that comes from the Hubbard model in the limit of infinite repulsion and one hole in a half-filled band [2]. Another example where saturated ferromagnetism has been shown to exist is the case of the one-dimensional Hubbard model with nearest and next-nearest-neighbor hopping at low electron densities [3]. Moreover, several examples of the fully polarized ground state have been found on special lattices (special conduction bands) as are the fcc-type lattices [4], the bipartite lattices with sublattices containing a different number of sites [5], the lattices with unconstrained hopping of electrons [6] and the flat bands [7]. This indicates that the lattice structure and the kinetic energy of electrons, i.e., the type of hopping play an important role in stabilizing the ferromagnetic state.

In this paper we show that if the electron hopping is described by a more realistic model (than the nearest-neighbor hopping) then ferromagnetism comes from the Hubbard model naturally for a wide range of the model parameters. No extra interactions terms should be included. In particular, we have found that the long-range hopping with power decaying hopping amplitudes t_{ij} given by [8]

$$t_{ij}(q) = \begin{cases} 0, & i = j, \\ -q^{|i-j|}/q, & i \neq j \end{cases} \tag{1}$$

gives rise to ferromagnetism for electron densities above half-filling. As soon as q that controls the effective range of the hopping ($0 \leq q \leq 1$) is different from zero the ferromagnetic state is stabilized for all Coulomb interactions U greater than some critical interaction strength $U_c(q)$ that value is dramatically reduced with increasing q. From this point of view one of main reasons why the ferromagnetic state absent in the ordinary Hubbard model with nearest-neighbor hopping ($q = 0$) is that the description of the electron hopping was too simplified.

The selection of hopping matrix elements in the form given by Eq. 1 has several advantages. It represents a much more realistic type of electron hopping on a lattice (in comparison to nearest-neighbor hopping), and it allows us to change continuously the type of hopping (band) from nearest-neighbor ($q = 0$) to infinite-range ($q = 1$) hopping and thus immediately study the effect of the long-range hopping. Another advantage follows from Fig. 1 where the density of states (DOS) corresponding to Eq. 1 is displayed for several values of q. It is seen that with increasing q more weight shifts to the upper edge of the band and the DOS becomes strongly asymmetric. Thus one can study simultaneously (by changing only one parameter q) the influence of the increasing asymmetry in the DOS and the influence of the long-range hopping on the ground state properties of the Hubbard model.

The Hamiltonian of the single-band Hubbard model is given by

$$H = \sum_{ij\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{2}$$

where $c^+_{i\sigma}$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron of spin σ at site i, $n_{i\sigma}$ is the corresponding number operator ($N_\sigma = \sum_i n_{i\sigma}$) and U is the

on-site Coulomb interaction constant.

The exact results on the ground states of the Hubbard model with the generalized type of hopping (Eq. 1) exist only for the special case of $q = 1$ when the electrons can hop to all sites with equal probabilities [6]. For this type of hopping and the electron filling just above half-filling ($N = \sum_\sigma N_\sigma = L + 1$, where L is the number of lattice sites) it was shown that the ground state is not degenerate with respect to the total spin S and it is maximally ferromagnetic with $S = (L - 1)/2$ (for all $U > 0$). For higher fillings ($N > L + 1$) the ferromagnetic ground state still exists but it is completely degenerate with respect to S. The limit of infinite-range hopping is, however, the least realistic limit of Eq. 1. It is interesting, therefore, to look at the possibility of ferromagnetism in the Hubbard model with a generalized type of hopping for smaller values of q that describe a much more realistic type of electron hopping.

In this paper we extend calculations to arbitrary q and arbitrary band fillings $n = N/L$. The ground states of the model are determined by exact diagonalizations for a wide range of model parameters (q, U, n). Typical examples are then chosen from a large number of available results to represent the most interesting cases. The results obtained are presented in the form of phase diagrams in the U-q plane. To determine the phase diagram in the U-q plane (corresponding to some L and n) the ground state energy of the model is calculated point by point as functions of q and U. Of course, such a procedure demands in practice a considerable amount of CPU time, which imposes severe restrictions on the size of clusters that can be studied with this method ($L \sim 16$). Fortunately, we have found that the ground-state energy of the model depends on L only very weakly (for a wide range of the model parameters) and thus already such small clusters can describe satisfactorily the ground state properties of the model.

Let us first briefly discuss the case of $N = L + 1$. According to analytical results [6] only for this case the ground state of the model with unconstrained hopping $q = 1$ is maximally ferromagnetic and nondegenerate with respect to the total spin S. Numerical calculations that we have performed on finite clusters up to $L = 12$ showed that the ferromagnetic state persists as the ground state also for $q < 1$, but with decreasing q the region of its stability shifts to higher values of U. In accordance with the exact results [6] obtained for $q = 1$ we found that the critical interaction strength $U_c(q)$ (above which the ground state is ferromagnetic) goes to zero for $q \to 1$ while in the opposite limit ($q \to 0$) U_c tends to infinity. Although the appearance of the ferromagnetic state at finite q and $N = L + 1$ is interesting from the theoretical point of view, thermodynamically this result is not significant if the ferromagnetic state does not persist also for higher fillings. Analytical results obtained for $q = 1$ predict, however, that the ground states for $N > L + 1$ are completely degenerate with respect to the total spin S and thus the only possibility for the stabilization of the ferromagnetic state is that the long-range hopping with $q \neq 1$ removes this degeneracy.

Numerical calculations that we have performed for a wide range of electron fillings $n > 1$ fully confirmed this assumption. It was found that the long-range hopping with $q \neq 1$ not only removes the degeneracy of the ground states with respect to S but at the same time stabilizes the ferromagnetic state. Furthermore, these calculations showed that the effect of the long-range hopping on the stability of the ferromagnetic state is extremely strong, especially for small values of q. The results of our small-cluster exact-diagonalization calculations obtained on finite clusters up to $L = 16$ sites are summarized in Fig. 2. There is shown the critical interaction strength U_c, above which the ground state is ferromagnetic, as a function of q for several values of electron concentrations n ($n = 5/4, 3/2, 7/4$). To

reveal the finite-size effects on the stability of ferromagnetic domains, the behavior of the critical interaction strength $U_c(q)$ has been calculated on several finite clusters at each electron filling. It is seen that finite-size effects on U_c are small and thus these results can be satisfactorily extrapolated to the thermodynamic limit $L \to \infty$. Our results clearly demonstrate that the ferromagnetic state is strongly influenced by q for electron concentrations above half-filling and generally it is stabilized with increasing q [9]. The effect is especially strong for small values of q where small changes of q reduce dramatically the critical interaction strength U_c and so the ferromagnetic state becomes stable for a wide range of model parameters. The results presented in Fig. 2d show that only for $q = 0$ (nearest-neighbor hopping) $U_c = \infty$, while for finite q (that represents a much more realistic type of electron hopping) the critical interaction strength U_c is finite. Thus the absence of ferromagnetism in the ordinary Hubbard model with the nearest-neighbor hopping ($q = 0$) can be explained as a consequence of too simplified description of electron hopping on the lattice. For any $q > 0$ ferromagnetism comes naturally from the Hubbard model with a generalized type of hopping for a wide range of model parameters without any other assumptions. This opens a new route towards the understanding of ferromagnetism in the Hubbard model.

In order to exclude the possibility that ferromagnetism in the Hubbard model with the long-range hopping described above is a consequence of boundary conditions used (open boundary conditions), let us finally examine the influence of boundary conditions on the stability of the ferromagnetic state. In Fig. 3 we present representative results of exhaustive numerical studies of the model obtained for $n = 3/2$ on all finite (even) clusters up to $L = 16$ sites for open and periodic boundary conditions. There is plotted the difference $\Delta E = E_f - E_g$ between the exact ground state E_g and the ferromagnetic state E_f as a function of

$1/U$ for $q = 0.25$ and different L. The ground state is ferromagnetic in the regions where $\Delta E = 0$. In accordance with results discussed above one can see a nice convergence of numerical results for the open boundary conditions. These results can be satisfactorily extrapolated to the thermodynamic limit $L = \infty$. We have plotted this extrapolated behavior in Fig. 3b to demonstrate clearly a convergence of small-cluster exact-diagonalization results for the periodic boundary conditions. It is seen that results for the periodic boundary conditions converge slowly than ones for the open boundary conditions, but their convergence to the thermodynamic limit is apparent. This confirms the stability of the ferromagnetic state in the Hubbard model with the long-range hopping.

In summary, the extrapolation of small-cluster exact-diagonalization calculations was used to examine ferromagnetism in the one-dimensional Hubbard model with a generalized type of hopping. It was found that the long-range hopping with power decaying hopping amplitudes stabilizes the ferromagnetic state for a wide range of model parameters. The critical value of the interaction strength $U_c(q)$ above which the ferromagnetic state becomes stable was calculated numerically and the ground-state phase diagram of the model (in the U-q plane) was presented for selected values of electron fillings.

This work was supported by the Slovak Grant Agency VEGA under grant No. 2/7021/20. Numerical results were obtained using computational resources of the Computing Centre of the Slovak Academy of Sciences.

References

[1] J. Hubbard, Proc. R. Soc. London A **276**, 238 (1963).

[2] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

[3] E. Múller-Hartmann, J. Low. Temp. Phys.**99**, 342 (1995).

[4] M. Ulmke, Eur. Phys. J. B **1**, 301 (1998).

[5] E.H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).

[6] P. Pieri, Mod. Phys. Lett. B**10**, 1277 (1996); M. Salerno, Z. Phys. B **99**, 469 (1996); *ibid.* B **101**, 619 (1996).

[7] A. Mielke and H. Tasaki, Commun. Math. Phys. **158**, 341 (1993).

[8] P. Farkašovský, J. Phys. Condens. Matter **7**, 3001 (1995); *ibid.* **7**, 9775 (1995); Phys. Rev. B **57**, 14722 (1998); Int. J. Mod. Phys. B **12**, 803 (1998).

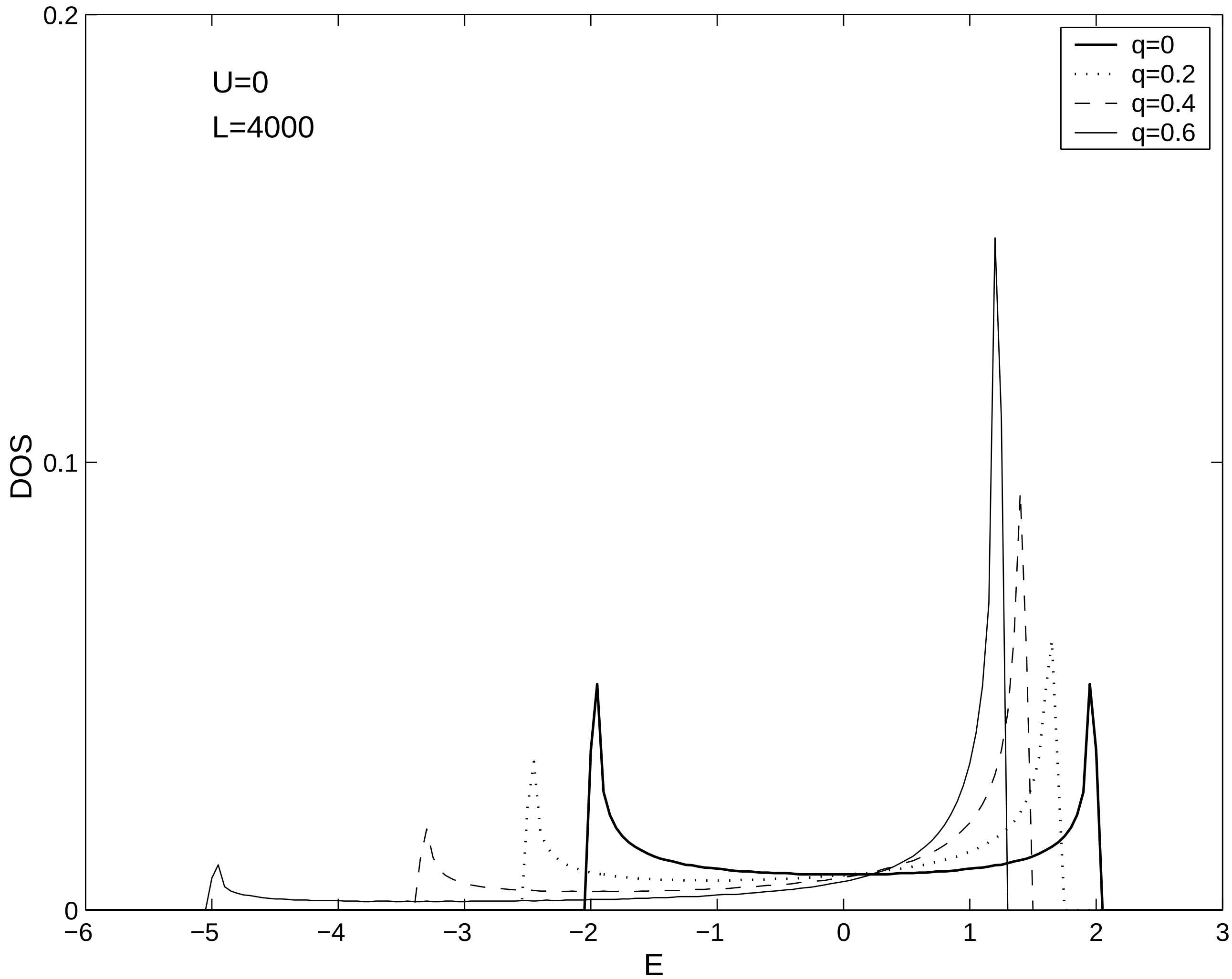
[9] In accordance with the analytical results (Ref. 6) we have found that the long-range hopping does not stabilize the ferromagnetic state for $n \leq 1$.

Figure Captions

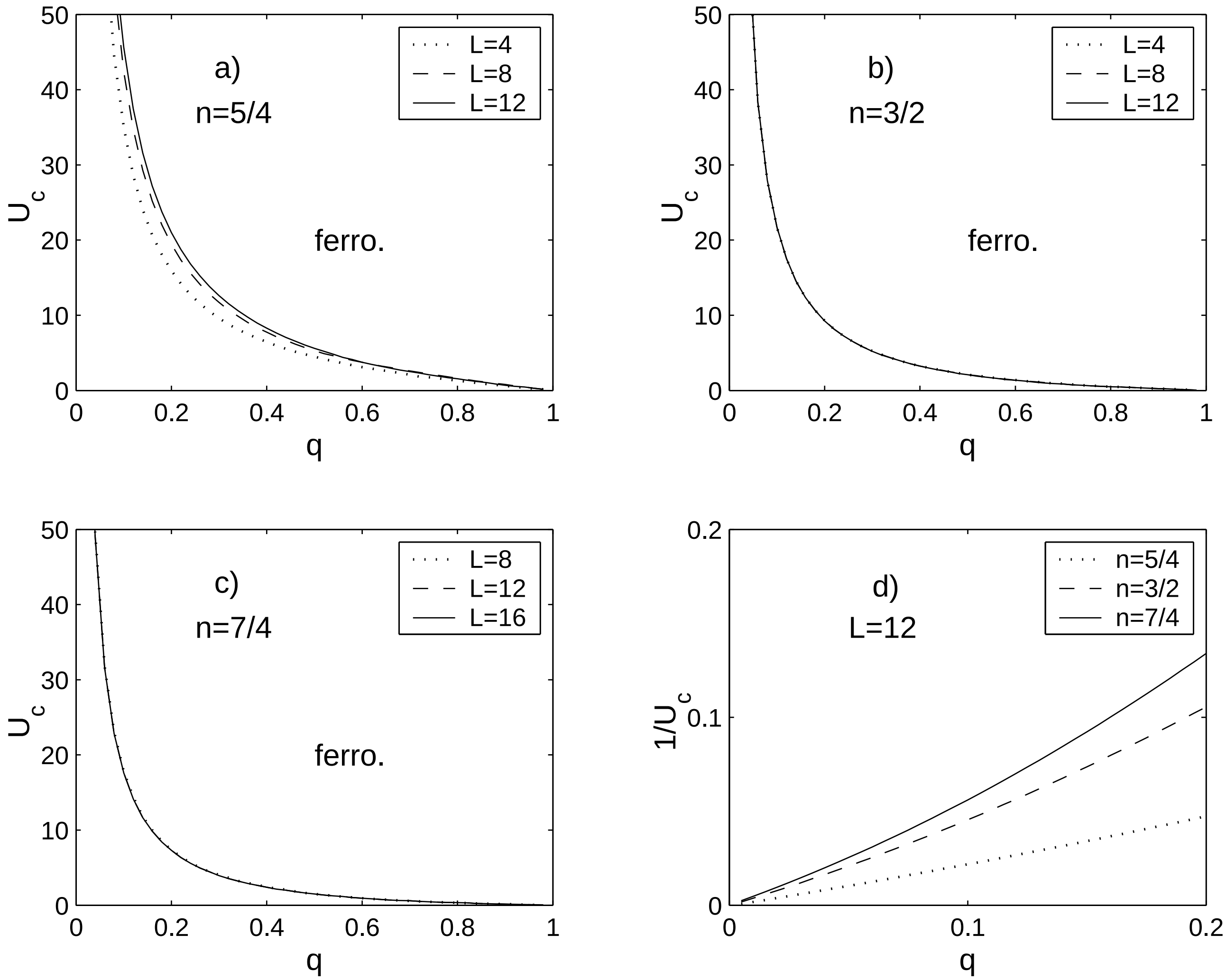
Fig. 1. The non-interacting DOS corresponding to a generalized hopping (Eq. 1) for different values of q and $L = 4000$ sites.

Fig. 2. The critical interaction strength U_c $(1/U_c)$ as a function of q calculated for different n and L.

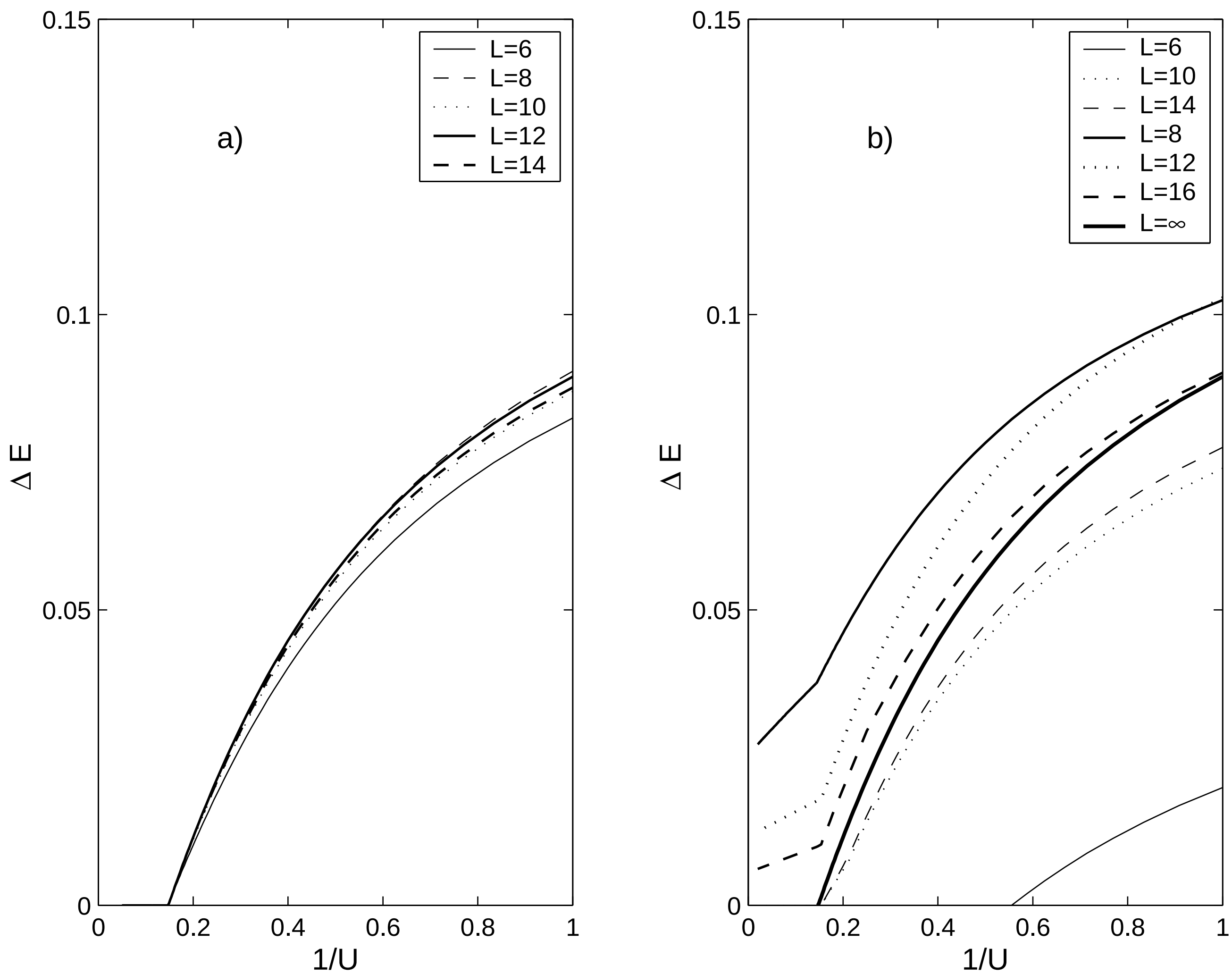
Fig. 3. The difference $\Delta E = E_g - E_f$ between the exact ground state E_g and the ferromagnetic state E_f as a function of $1/U$ calculated for $n = 3/2, q = 0.25$ and different L. (a) Open boundary conditions. (b) Periodic boundary conditions.



U=0
L=4000
q=0
q=0.2
q=0.4
q=0.6
DOS
E
0.2
0.1
0
−6
−5
−4
−3
−2
−1
0
1
2
3



a)
n=5/4
L=4
L=8
L=12
ferro.
U_c
q
b)
n=3/2
L=4
L=8
L=12
ferro.
U_c
q
c)
n=7/4
L=8
L=12
L=16
ferro.
U_c
q
d)
L=12
n=5/4
n=3/2
n=7/4
1/U_c
q


a)
L=6
L=8
L=10
L=12
L=14
ΔE
1/U
0.15
0.1
0.05
0
0
0.2
0.4
0.6
0.8
1
b)
L=6
L=10
L=14
L=8
L=12
L=16
L=∞
ΔE
1/U